Seminario de Estudiantes 2018-B

Invita a la séptima plática del periodo Otoño 2018

"A computational screening of alkali metal-halide, inorganic perovskites for solar cell applications"

Presenta

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RESUMEN

In recent years, solution-processed organic–inorganic metal halide perovskites have become some of the most notable materials owing to its beneficial impact on solar cells efficiency. However, organic halide perovskites suffer from chemical instability in the presence of water, oxygen and under illumination, especially at high temperatures. In this regard, all-inorganic metal halide perovskites have become an interesting alternative to the hybrid counterpart, because of the superior stability and comparable electronic structure and related properties such as tunable band gap, strong emission, and high fluorescence quantum yield. Therefore, one of the main challenges in this research field is to find environmentally friendly and highly efficiently perovskites for solar energy applications. In order to guide such quest, in this work we present a computational study on the family of alkali metal-halide inorganic perovskites AMX3 (A=Cs, Rb, K, Na, Li; M=Pb, Sn, Ge, Si; X=I, Br, Cl, F), by means of density functional theory (DFT) calculations. Because the temperature dependence of the structural properties in such perovskites is well-known, we studied each compound in the cubic, tetragonal, orthorhombic, trigonal, monoclinic, and the so-called yellow phases. The electronic band gaps were computed within the DFT-1/2 correction, including spin-orbit coupling effects. We present a computational screening of the best candidates for high solar cell efficiency, in terms of the structural and electronic properties of the studied perovskites.

Keywords: Inorganic halide perovskites, Solar energy materials, Computational screening

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